



3 1176 00166 6388

NASA Technical Memorandum 81710

NASA-TM-81710 19810017243

# The Self-Consistent Calculation of Pseudomolecule Energy Levels, Construction of Energy Level Correlation Diagrams and an Automated Computational System for SCF- $X\alpha$ -SW Calculations

Herbert Schlosser  
*Lewis Research Center*  
*Cleveland, Ohio*

LIBRARY COPY

JUN 25 1981

LEWIS RESEARCH CENTER  
LIBRARY, NASA  
CLEVELAND, OHIO

March 1981

**NASA**



## SUMMARY

This work is concerned with the self-consistent calculation of the electronic energy levels of noble gas pseudomolecules formed when a metal surface is bombarded by noble gas ions and with the construction of energy level correlation diagrams as a function of interatomic spacing. The self-consistent-field  $x\alpha$  scattered wave (SCF- $x\alpha$ -SW) method of Slater and Johnson is utilized. Preliminary results on the Ne-Mg system are given.

An interactive  $x\alpha$  programming system, which has been implemented on the LeRC IBM 370 computer, is described in detail. This automated system makes use of special PROCDEFS (procedure definitions) to minimize the data to be entered manually at a remote terminal. Listings of the special PROCDEFS and of typical input data are given.

## INTRODUCTION

Ferrante and Pepper (ref. 1) recently investigated Auger electron production by  $\text{Ne}^+$  bombardment of Mg, Al, and Si surfaces. Ion energies in the range of 1-3 KeV were used. Auger electrons characteristic of both the target atoms and the incident Ne were observed. They attributed these observations to asymmetric Ne-surface atom collisions, and presented evidence that the Auger electrons resulted from autoionization of neutral, excited Ne. Their results on the variation in strength of Ne Auger signals with target in the sequence Mg, Al, Si appear to be in agreement with the predictions of the electron-promotion excitation mechanism of Barat and Lichten (ref. 2). Ferrante and Pepper (ref. 3) have also investigated the production of Auger electrons by bombardment of Mg and Al surfaces with other noble gas ions. To help elucidate the question of electron-promotion in the formation of collision-induced pseudomolecules, it is of great interest to obtain accurate energy level correlation diagrams for the pseudomolecules formed from various noble gas-metal pairs. In the present paper the results of a preliminary calculation of a Ne-Mg correlation diagram using the  $x\alpha$  method are presented. In addition, a description of the  $x\alpha$  program, which can be used for a wide variety of chemical and solid state calculation, is presented to facilitate its use by interested parties at LeRC.

Professor J. G. Norman, Jr., of the University of Washington, supplied basic  $x\alpha$  programs and operating instructions.

## SELF-CONSISTENT CALCULATION OF PSEUDOMOLECULE ENERGY LEVELS, CONSTRUCTION OF CORRELATION DIAGRAMS

This work is concerned with the self-consistent calculation of the energy levels of noble gas-metal pseudomolecules formed when a metal surface is bombarded by noble gas ions, and with the construction of energy level correlation diagrams. The theoretical method utilized in the molecular calculations is the self-consistent-field  $x\alpha$  scattered-wave (SCF- $x\alpha$ -SW) method of Slater and Johnson (ref. 4). The interactive  $x\alpha$  programing system described in the following section was implemented on the LeRC IBM 370-3033 computer for this purpose. To construct a correlation diagram for a particular system, electronic energy levels must be calculated for a number of different interatomic spacings ranging from the separated atom to the united atom limits. The atomic calculations were performed using the modified Herman Skillman SCF program described below (ref. 5). Preliminary results on the Ne-Mg system are summarized in figure 1.

In the usual application of the  $x\alpha$ -SW method, the molecule is surrounded by a sphere, and the interior is partitioned into a number of spherical atomic regions and an interatomic region. The molecular potential is constructed to be spherically symmetric in the atomic and extra molecular regions and constant in the interatomic region. The Schrodinger equation is then solved self-consistently, subject to the boundary condition that the wave function and its first derivative are continuous across all boundaries, using the multiple scattering formalism combined with the  $x\alpha$  density function formalism for treating the exchange and correlation. In general, the iterative self-consistent field computational scheme is reasonably rapidly convergent. In the earliest applications of the  $x\alpha$ -MS method, the atomic spheres were taken as non-overlapping. As larger and more "open" systems were investigated, the constant potential interatomic regions become an appreciable portion of the molecular volume, and convergence difficulties were found. This was remedied empirically by allowing the atomic spheres to overlap each other. Consequently, the theory was reformulated for the case of overlapping spheres. The major constraint on the use of overlapping atomic spheres is that the spheres may not overlap any adjacent atomic center. Thus, the largest allowable sphere for a given atomic center is slightly less than the nearest neighbor distance. In the present calculations, the use of overlapping spheres is essential, particularly for the small interatomic distances ( $r < 2\text{AU}$ ) in the pseudomolecules formed at the projectile energies used in the experiments. The projectile energy range of interest in Ne-Mg (1-3 KeV) corresponds to interatomic distances in the range 0.47 AU to about 1.0 AU (ref. 6).

## INTERACTIVE SCF- $x\alpha$ -SW CALCULATIONS

The computer programs necessary to carry out SCF- $x\alpha$ -SW calculations in an interactive manner have been implemented on the LeRC IBM 370 computer using the TSS operating system. In order to facilitate use of the programs interactively from a terminal, and to minimize the amount of data to be entered from the terminal, a series of special PROCDEFS (procedure definitions) were created (appendix I). The use of these are demonstrated below. A complete  $x\alpha$  calculation entails the following sequence of steps, each of which involves the use of a different program package:

- (a) Generation of atomic potentials for each atom or ion in the molecule using a modified Herman Skillman SCF program
- (b) Generation of a molecular potential by superposition of atomic potentials
- (c) Generation of a contracted molecular potential for use in steps (e) and (f)
- (d) Generation of symmetry input for use in steps (e) and (f)
- (e) Calculation of the energy levels of the molecule
- (f) SCF calculation starting with the results of step (e) plus subsequent iteration

In addition, one may calculate the wave functions and charge densities corresponding to the SCF energy levels and also plot these quantities. (Thus far, these programs have not been implemented.) The output from each successive step is stored in a specified element on disk. The programs for each successive step are run under the control of an appropriate PROCDEF. The input data for a given step is automatically constructed by the PROCDEF by combining the previously stored elements with minimal input entered from the terminal.

To illustrate the use of the PROCDEFS referred to above, we shall consider the sequence of operations involved in carrying out an SCF calculation for a Mg-Ne pseudomolecule.

### A. Generation of atomic potentials

The format of the input data cards necessary to generate atomic potentials using the modified Herman Skillman program are described in the unpublished operating instructions for the  $x\alpha$  programs. A listing of the input cards for Ne, stored in element NEI, is given in appendix II(B). To generate the atomic potential for Ne and to store the card image output in element NEI, one enters

```
_HSRUN NEI, NE1
```

at the terminal. The terminal will respond with

```
DDNAME FT06F001 UNDEFINED ENTER Y. . . .
```

To print the condensed tabular output at the terminal, one enters D. The eigenvalues for each iteration, and the total charge density and core charge density for the final iteration are then printed at the terminal. Card image output is stored in element NE1.

#### B. Generation of molecular potential

The input data cards for a Ne-Mg pseudomolecule, stored in element NEMG, are listed in appendix II(C). The cards are for the case where the Ne atom has coordinates (2, 0, 0) AU and Mg (-2, 0, 0) AU. To run the program, one enters

```
_MRUN NEMG, VNM
```

at the terminal. The PROCDEF loads NEMG and goes into the edit mode now assuming that the Ne and Mg total and core charge densities are stored in Ne1 and MG1, respectively, one next types in

```
B; LOA NE1; B; LOA MG1
```

This loads NE1 and MG1. To reenter the PROCDEF and to continue the calculation, one types

```
_DEFAULT SYSINX=E
```

The output molecular potential is stored in element VNM. For this program tabular output is listed on the high-speed printer, rather than at the terminal, because the output is quite lengthy (2200 lines for NeMg).

#### C. Generation of contracted molecular potential

The next step is the generation of a contracted molecular potential assuming specific values of radii for the atomic and outer spheres in the molecule. If the input molecular potential is stored in element VNM, the contracted potential is to be stored in VVM and the radii of the outer, Ne, Mg spheres are 0.705, 0.4332, 0.470 AU, respectively, one enters at the terminal:

```
_CRUNT VNM, VVM
```

```
I .705 .4332 .47 0.0
```

```
_DEFAULT SYSINX = E
```

The terminal responds with

```
DDNAME FT06F001 UNDEFINED. . . .
```

Upon entry of D, the calculation proceeds and tabular output is printed at the terminal. The table of the output contracted molecular potential is listed in appendix II(E).

#### D. Generation of symmetry input

This program calculates spherical harmonic basis functions for a given set of  $l$  values, and writes out card images which are stored in a specified element. The calculation must be repeated for each unique group of equivalent atoms and each symmetry group. The output elements must then be edited to form the input for E and F. Suppose the required input cards, described in the  $x\alpha$  operating instructions, have been placed in element PIN and the output element name is PIO. One would enter

```
_YLRUN PIN,PIO
```

at the terminal, which then responds with

```
DDNAME FT06001 UNDEFINED. . . .
```

Upon entry of D, the calculation proceeds and tabular output is printed at the terminal. The final edited versions of the symmetry output for the  $\sigma$ ,  $\pi$  representations of the group of the heteronuclear diatomic molecule are given in appendix II(A).

#### E. Energy level calculation

Suppose that one wishes to search for energy levels in the energy range  $-0.5$  AU to  $-10.$  AU in steps of  $0.5$  AU. One would enter

```
_FRUN VNM,PIZ
```

at the terminal. (The contracted potential is stored in element VNM, and the symmetry input is stored in PIZ.) The terminal will respond with

```
DDNAME FT06F001 UNDEFINED. . . .
```

and one enters D to print tabular output at the terminal. When the terminal indicated the editor is entered, one types in

```
I 3,1,.5,-.5,-10.,0
```

```
DEFAULT SYSINX=E
```

and the calculation proceeds. The determinant value for each trial energy in the range specified is then calculated and printed. If the sign of the determinant changes in a

given energy range, the program automatically interpolates for the energy corresponding to zero determinant (that is, energy eigenvalue).

#### F. SCF calculation

The final step in the  $x\alpha$  calculational procedure is the iterative SCF calculation. This is performed in two stages under control of two different PROCDEFs. In the first stage, the necessary input data for the second stage is constructed automatically by the PROCDEF. This is convenient because of the complexity of the input data and because similar input data is needed for the SCF calculations at different interatomic distances. The PROCDEF DIS constructs SCF input for NeMg in the case where there are 4 different sigma levels and 2 different pi levels occupied in the pseudomolecule. One must also specify the number of iterations to be performed and the energies of the frozen core levels. Suppose the number of iterations desired is 8, frozen core levels are found at -60.9204, -92.6720 AU, sigma states at -6.30841, -4.51048, -2.88924 -1.46411 AU, and pi states at -3.63858 and -1.601967. One enters at the terminal

```
DIG 8, -60.9204, -92.6720, -6.30841, -4.51048,  
-2.88924, -1.46411, -3.63858, -1.601967
```

This generates the SCF input, placing it in element DIG. The SCF input generated for this case is listed in appendix II(F). Next, with input potential in VM and output in VM1, the SCF step is started by typing

```
_SCFR VM, DIG, VM1
```

The terminal responds with

```
DDNAME FT06F001 UNDEFINED. . . . .,
```

and one enters D to proceed. In each iteration the input levels and occupation numbers, the various components of potential energy, the total potential energy, kinetic energy, total energy and virial coefficient are printed. Also printed are the total charge in each region, the largest difference between the old and new potentials, calculated energy eigenvalues for the old potential, and predicted eigenvalues for the new potential. After the last iteration, charges are given as fractions of the total charge within the atomic spheres, and decomposed in their spherical-harmonic (s, p, d, f, etc.) components. Finally, the new potential is printed at the terminal.



## APPENDIX I - PROCDEFS FOR RUNNING THE X $\alpha$ PROGRAMS

### A. HERMAN SKILLMAN ATOMIC POTENTIAL PROCDEF

```
LIST 0,1000
HSRUN 0000000 PROCDEF HSRUN
HSRUN 0000100 PARAM TN,OUT
HSRUN 0000150 DEFAULT SYSINX=E
HSRUN 0000200 IN
HSRUN 0000300 %E
HSRUN 0000400 REDIT TN
HSRUN 0000500 B:LOA INPU;VS INPU;Q
HSRUN 0000600 HRUN HSKK,OUT
HSRUN 0000700 ABEND
```

```
PROCDEF HRUN
LIST 100,2500
HRUN 0000100 PARAM JBLIB,CARD
HRUN 0000200 PPLI
HRUN 0000300 DDEF ASD,VP,JBLIB,OPTION=JOB LIB
HRUN 0000400 FILEDEF FT05F001,VS,INPU,DCB=(RECFM=F,LRECL=80)
HRUN 0000500 FILEDEF FT07F001,VS,CARD,DCB=(RECFM=F,LRECL=80)
HRUN 0000600 QSRUN MAIN
HRUN 0000700 PRINT CARD
HRUN 0000800 FILEREL FT05F001,FT07F001
HRUN 0000900 ERASE INPU
HRUN 0001000 RELEASE ASD
```

### B. MOLECULAR POTENTIAL PROCDEF

```
PROCDEF MRUN
LIST 100,2500
MRUN 0000100 PARAM TNP,OUT
MRUN 0000200 DEFAULT SYSINX=E
MRUN 0000300 IN
MRUN 0000400 %E
MRUN 0000500 REDIT TNP
MRUN 0000600 PAUSE
MRUN 0000700 DEFAULT SYSINX=G
MRUN 0000800 CONEDIT
MRUN 0000900 B:LOA INPU;VS INPU
MRUN 0001000 Q
MRUN 0001100 SRUN MOLE,OUT
MRUN 0001200 ABEND
```

```

PROCDEF SRUN
LIST 100,2500
SRUN      0000100  PARAM JLIB,CARD
SRUN      0000200  PPLI
SRUN      0000300  FILEDEF FT06F001,VS,OUT,DCB=(RECFM=F,LRECL=136),RET=T
SRUN      0000400  HRUN JLIB,CARD
SRUN      0000500  PRINT OUT
SRUN      0000600  FILEREL FT06F001

```

```

PROCDEF HRUN
LIST 100,2500
HRUN      0000100  PARAM JBLIB,CARD
HRUN      0000200  PPLI
HRUN      0000300  DDEF ASD,VP,JBLIB,OPTION=JOBLIB
HRUN      0000400  FILEDEF FT05F001,VS,INPU,DCB=(RECFM=F,LRECL=80)
HRUN      0000500  FILEDEF FT07F001,VS,CARD,DCB=(RECFM=F,LRECL=80)
HRUN      0000600  OSRUN MAIN
HRUN      0000700  PRINT CARD
HRUN      0000800  FILEREL FT05F001,FT07F001
HRUN      0000900  ERASE INPU
HRUN      0001000  RELEASE ASD

```

### C. CONTRAC PROCDEF

```

PROCDEF CRUNT
LIST 100,2500
CRUNT     0000100  PARAM TNP',OUT
CRUNT     0000200  DEFAULT SYSINX=E
CRUNT     0000300  IN
CRUNT     0000400  %E
CRUNT     0000500  REDIT TNP'
CRUNT     0000600  T;LOA RNEMG;T;N 2;D
CRUNT     0000700  PAUSE
CRUNT     0000800  DEFAULT SYSINX=G
CRUNT     0000900  CONEDIT
CRUNT     0001000  B;LOA INPU;VS INPU;Q
CRUNT     0001100  HRUN CONT,OUT
CRUNT     0001200  REDIT OUT
CRUNT     0001300  T;P 1000;Q
CRUNT     0001400  ABEND

```

```

PROCDEF HRUN
LIST 100,2500
HRUN      0000100  PARAM JBLIB,CARD
HRUN      0000200  PPLI
HRUN      0000300  DDEF ASD,VP,JBLIB,OPTION=JOBLIB
HRUN      0000400  FILEDEF FT05F001,VS,INPU,DCB=(RECFM=F,LRECL=80)
HRUN      0000500  FILEDEF FT07F001,VS,CARD,DCB=(RECFM=F,LRECL=80)
HRUN      0000600  OSRUN MAIN
HRUN      0000700  PRINT CARD
HRUN      0000800  FILEREL FT05F001,FT07F001
HRUN      0000900  ERASE INPU
HRUN      0001000  RELEASE ASD

```

#### D. SYMMETRIZATION PROGRAM PROCDEF

```

PROCDEF YLRUN
LIST 100,1500
YLRUN     0000100  PARAM YLIN,OUT
YLRUN     0000200  DEFAULT SYSINX=E
YLRUN     0000210  IN
YLRUN     0000220  %E
YLRUN     0000300  REDIT YLIN
YLRUN     0000400  B;LOA INPU;VS INPU;Q
YLRUN     0000500  PPLI
YLRUN     0000600  TTPE FT08F001,SCR
YLRUN     0000700  HRUN HAR,OUT
YLRUN     0000800  FILEREL FT08F001
YLRUN     0000900  REDIT OUT
YLRUN     0001000  T;P 300;Q
YLRUN     0001100  ABEND

```

```

PROCDEF HRUN
LIST 100,1900
HRUN      0000100  PARAM JBLIB,CARD
HRUN      0000200  PPLI
HRUN      0000300  DDEF ASD,VP,JBLIB,OPTION=JOBLIB
HRUN      0000400  FILEDEF FT05F001,VS,INPU,DCB=(RECFM=F,LRECL=80)
HRUN      0000500  FILEDEF FT07F001,VS,CARD,DCB=(RECFM=F,LRECL=80)
HRUN      0000600  OSRUN MAIN
HRUN      0000700  PRINT CARD
HRUN      0000800  FILEREL FT05F001,FT07F001
HRUN      0000900  ERASE INPU
HRUN      0001000  RELEASE ASD

```

```

PROCDEF TTPE
LIST 100,1300
TTPE      0000100  PARAM TAPE,SCRAT
TTPE      0000200  FILEDEF TAPE,VS,SCRAT,DCB=(RECFM=V,LRECL=800),OSRECFM=VS,RET=T

```

## E. ENERGY CALCULATION PROCDEF

```
PROCDEF FRUN
LIST 100,1900
FRUN      0000100  PARAM NAME,DIA
FRUN      0000200  DEFAULT SYSINX=E
FRUN      0000300  IN
FRUN      0000400  %E
FRUN      0000500  REDIT NAME
FRUN      0000550  T:I ENERGY
FRUN      0000600  B:LOA DIA:B
FRUN      0000700  PAUSE
FRUN      0000800  DEFAULT SYSINX=G
FRUN      0000900  CONEDIT
FRUN      0001000  I 0,0,0,0,0,0
FRUN      0001100  B:LOA INPU;VS INPU;Q
FRUN      0001200  YRUN ENER,ENEI
FRUN      0001300  ABEND
```

```
PROCDEF YRUN
LIST 100,1900
YRUN      0000100  PARAM JBLIB,CARD
YRUN      0000200  PPLI
YRUN      0000300  DDEF ASD,VP,JBLIB,OPTION=JOBLIB
YRUN      0000400  DDEF BSD,VP,NJLIB,OPTION=JOBLIB
YRUN      0000450  DDEF CSD,VP,TMA,OPTION=JOBLIB
YRUN      0000500  FILEDEF FT05F001,VS,INPU,DCB=(RECFM=F,LRECL=80)
YRUN      0000600  FILEDEF FT07F001,VS,CARD,DCB=(RECFM=F,LRECL=80)
YRUN      0000700  OSRUN MAIN
YRUN      0000800  PRINT CARD
YRUN      0000900  FILEREL FT05F001,FT07F001
YRUN      0001000  ERASE INPU
YRUN      0001100  RELEASE ASD
YRUN      0001200  RELEASE BSD
YRUN      0001300  RELEASE CSD
```

## F. PROCDEF FOR GENERATING SCF PROGRAM INPUT

```
PROCDEF DIS
LIST 0,1000
DIS       0000000  PROCDEF DIS
DIS       0000100  PARAM NUM,N1,M1,A1,B1,C1,D1,E1,F1
DIS       0000200  DEFAULT SYSINX=E
DIS       0000250  ERASE RIG
DIS       0000300  REDIT DIG
DIS       0000400  PD 200;C /8/NUM/;N;DU 12/N1/;P;N;DU 12/M1/;P;N;DU 11/A1/;
P;PD 2300;DU 11/B1/;P;N;DU 11/C1/;P;N
DIS       0000500  DU 11/D1/;P;N;DU 11/E1/;P;B;DU 11/F1/;P;FIL RIG;Q
DIS       0000600  ABEND
```

## G. SELF-CONSISTENT FIELD CALCULATION

```
PROCDEF SCFR
LIST 100,3000
SCFR 0000100 PARAM NAME,DIA,SCFOT
SCFR 0000200 DEFAULT SYSINX=E
SCFR 0000250 ERASE INPU
SCFR 0000300 IN
SCFR 0000350 SCF
SCFR 0000400 %E
SCFR 0000500 REDIT DIA
SCFR 0000600 PO 100;LOA NAME;N;D;B
SCFR 0001000 I 0,0,0,0,0,0
SCFR 0001100 T;LOA INPU;VS INPU;Q
SCFR 0001200 XRUN SCFOT
SCFR 0001400 REDIT SCFOT
SCFR 0001450 T;I 1 1
SCFR 0001500 T;P 1000;FIL SCFOT
SCFR 0001600 PAUSE
SCFR 0001700 DEFAULT SYSINX=G
SCFR 0001750 CONEDIT
SCFR 0001800 FIL SCFOT;Q
SCFR 0001900 ABEND
```

```
PROCDEF XRUN
LIST 100,2500
XRUN 0000100 PARAM CARD
XRUN 0000200 PPLI
XRUN 0000300 DDEF ASD,VP,ENER,OPTION=JOBLIB
XRUN 0000310 DDEF BSD,VP,NJLIB,OPTION=JOBLIB
XRUN 0000320 DDEF DSD,VP,TMA,OPTION=JOBLIB
XRUN 0000355 DDEF CSD,VP,SCFL,OPTION=JOBLIB
XRUN 0000360 TTPE FT08F001,SC8
XRUN 0000365 TTPE FT10F001,SC0
XRUN 0000370 TTPE FT11F001,SC1
XRUN 0000375 TTPE FT12F001,SC2
XRUN 0000380 TTPE FT13F001,SC3
XRUN 0000500 FILEDEF FT05F001,VS,INPU,DCB=(RECFM=F,LRECL=80)
XRUN 0000600 FILEDEF FT07F001,VS,CARD,DCB=(RECFM=F,LRECL=80)
XRUN 0000700 OSRUN MAIN
XRUN 0000800 FILEREL FT
XRUN 0001000 ERASE INPU
XRUN 0001100 RELEASE ASD
XRUN 0001200 RELEASE BSD
XRUN 0001300 RELEASE CSD
XRUN 0001400 RELEASE DSD
```

```
PROCDEF TTPE
LIST 100,1200
TTPE 0000100 PARAM TAPE,SCRAT
TTPE 0000200 FILEDEF TAPE,VS,SCRAT,DCB=(RECFM=V,LRECL=800),OSRECFM=VS,RET=T
```

# APPENDIX II - INPUT DATA FOR THE X $\alpha$ PROGRAMS

## A. DIATOMIC MOLECULE SYMMETRY INPUT FOR ENERGY, SCF CALCULATIONS

REDIT PIZ  
LOADING PIZ  
EDIT

TiP 100;Q

	TOP	RECORD	PI	Z	REP
0000020	10	2			
0000200	1	1			
0000300	0	1	1		1.00000000
0000400	2	1			
0000500	1	1	1		1.00000000
0000600	3	1			
0000700	0	1	1		1.00000000
0000800	3	1			
0000900	2	1	1		1.00000000
0001000	4	1			
0001100	1	1	1		1.00000000
0001200	4	1			
0001300	3	1	1		1.00000000
0001500	1	1			
0001600	0	1	2		1.00000000
0001700	2	1			
0001800	1	1	2		1.00000000
0002000	1	1			
0002100	0	1	3		1.00000000
0002200	2	1			
0002300	1	1	3		1.00000000

EDF

REDIT SIGMA  
LOADING SIGMA  
EDIT

TiP 100;Q

	TOP	RECORD	SIGMA	REP
0000020	8	2		
0000200	0	1		
0000300	0	1	1	1.00000000
0000400	1	1		
0000500	1	1	1	1.00000000
0000600	2	1		
0000700	0	1	1	1.00000000
0000800	2	1		
0000900	2	1	1	1.00000000
0002100	0	1		
0002200	0	1	2	1.00000000
0002300	1	1		
0002400	1	1	2	1.00000000
0003000	0	1		
0003100	0	1	3	1.00000000
0003200	1	1		
0003300	1	1	3	1.00000000

EDF

## B. NEI: HERMAN SKILLMAN PROGRAM NE INPUT

```

0000100 CONT      PUNC
0000120          NEUTRAL NEON ATOMIC POTENTIAL ; 15 FROZEN
0000200      0 .001 .00001 441 1 50 1 .73081
0000300      1.00 .99205 .98387 .97552 .96705 .95850 .94990 .94128 .93266 .92407
0000400      .91553 .89862 .88202 .86578 .84994 .83451 .81947 .80484 .79058 .77670
0000500      .76316 .73706 .71215 .68835 .66558 .64381 .62303 .60322 .58438 .56648
0000600      .54948 .51795 .48923 .46280 .43822 .41523 .39363 .37332 .35422 .33627
0000700      .31941 .28880 .26198 .23853 .21805 .20015 .18447 .17068 .15851 .14773
0000800      .13812 .12180 .10847 .1 .1 .1 .1 .1 .1 .1
0000900      .1 .1 .1 .1 .1 .1 .1 .1 .1 .1
0001000      .1 .1 .1 .1 .1 .1 .1 .1 .1 .1
0001100      .1 .1 .1 .1 .1 .1 .1 .1 .1 .1
0001200      .1 .1 .1 .1 .1 .1 .1 .1 .1 .1
0001300      .1 .1 .1 .1 .1 .1 .1 .1 .1 .1
0001400      10 1 2
0001500      100 2. -60.92
0001600      200 2. -3.168
0001700      210 6. -1.471
0001800

```

## C. NEMG: INPUT FOR MOLEC PROGRAM (NE-MG)

```

0000100      1
0000200      3 3 1 PCH PRT 1 .73
0000300 OUT 0 2 1 0. 0. .73
0000400      2 1 2 3 1 3
0000500 NE 0 1 2 2. 0. 0. .73081
0000600      3 1 3
0000700 MG 0 1 3 -2. 0. 0. .72913
0000800      2 1 2

```

## D. RNEMG: CONTRAC INPUT FOR NE-MG

```

0000100      2 2
0000120 4.946 2.14942 2.946 0.
0000300 0.
0000400 0.
0000500 0.

```

## E. VVM: CONTRACTED MOLECULAR POTENTIAL

(INPUT FOR ENERGY, SCF PROGRAMS)

```

      1 1 0.0 0.0
      3 3 1 2 0.73000 1 2
OUT 0 1 0 93 4 0.0 0.0 0.0 0.70500 0.73000
      22 42 62 82 102 122 142 162 182 202
0.5843213E+00 0.6197348E+00 0.6551484E+00 0.6905621E+00 0.7259757E+00
0.7613893E+00 0.7968029E+00 0.8322166E+00 0.8676302E+00 0.9030438E+00
0.9384574E+00 0.9738711E+00 0.1009284E+01 0.1044696E+01 0.1080108E+01
0.1115520E+01 0.1150931E+01 0.1186343E+01 0.1221755E+01 0.1257167E+01
0.1292579E+01 0.1327991E+01 0.1398816E+01 0.1469642E+01 0.1540467E+01
0.1611293E+01 0.1682118E+01 0.1752944E+01 0.1823770E+01 0.1894595E+01
0.1965421E+01 0.2036246E+01 0.2107072E+01 0.2177897E+01 0.2248723E+01

```

0.2319549E+01	0.2390374E+01	0.2461200E+01	0.2532025E+01	0.2602851E+01	11
0.2673676E+01	0.2744502E+01	0.2886155E+01	0.3027808E+01	0.3169461E+01	12
0.3311114E+01	0.3452767E+01	0.3594420E+01	0.3736073E+01	0.3877727E+01	13
0.4019380E+01	0.4161033E+01	0.4302686E+01	0.4444339E+01	0.4585992E+01	14
0.4727645E+01	0.4869298E+01	0.5010951E+01	0.5152604E+01	0.5294257E+01	15
0.5435910E+01	0.5577563E+01	0.5860871E+01	0.6144179E+01	0.6427487E+01	16
0.6710795E+01	0.6994103E+01	0.7277411E+01	0.7560719E+01	0.7844028E+01	17
0.8127336E+01	0.8410644E+01	0.8693952E+01	0.8977260E+01	0.9260568E+01	18
0.9543876E+01	0.9827184E+01	0.1011049E+02	0.1039380E+02	0.1067711E+02	19
0.1096042E+02	0.1124372E+02	0.1181034E+02	0.1237696E+02	0.1294358E+02	20
0.1351020E+02	0.1407681E+02	0.1464343E+02	0.1521005E+02	0.1577667E+02	21
0.1634326E+02	0.1690985E+02	0.1747644E+02			22
-0.2463831E+02	-0.2177068E+02	-0.1933852E+02	-0.1725706E+02	-0.1546275E+02	23
-0.1390690E+02	-0.1255136E+02	-0.1136551E+02	-0.1032433E+02	-0.9407094E+01	24
-0.8596468E+01	-0.7877851E+01	-0.7238875E+01	-0.6669029E+01	-0.6159349E+01	25
-0.5702175E+01	-0.5290941E+01	-0.4920012E+01	-0.4584542E+01	-0.4280350E+01	26
-0.4003827E+01	-0.3751849E+01	-0.3311037E+01	-0.2940171E+01	-0.2625712E+01	27
-0.2357213E+01	-0.2126528E+01	-0.1927226E+01	-0.1754170E+01	-0.1603210E+01	28
-0.1470954E+01	-0.1354603E+01	-0.1251829E+01	-0.1160684E+01	-0.1079531E+01	29
-0.1006984E+01	-0.9418747E+00	-0.8832099E+00	-0.8301487E+00	-0.7819747E+00	30
-0.7380802E+00	-0.6979455E+00	-0.6272457E+00	-0.5670267E+00	-0.5151748E+00	31
-0.4700947E+00	-0.4305671E+00	-0.3956457E+00	-0.3645864E+00	-0.3367962E+00	32
-0.3117971E+00	-0.2892004E+00	-0.2686865E+00	-0.2499905E+00	-0.2328922E+00	33
-0.2172046E+00	-0.2027718E+00	-0.1894593E+00	-0.1771549E+00	-0.1657573E+00	34
-0.1551822E+00	-0.1453576E+00	-0.1276935E+00	-0.1123301E+00	-0.9892082E-01	35
-0.8718550E-01	-0.7689518E-01	-0.6785882E-01	-0.5991211E-01	-0.5291684E-01	36
-0.4675342E-01	-0.4132001E-01	-0.3653039E-01	-0.3230766E-01	-0.2858673E-01	37
-0.2529121E-01	-0.2237942E-01	-0.1980313E-01	-0.1755022E-01	-0.1554865E-01	38
-0.1377345E-01	-0.1221491E-01	-0.9601045E-02	-0.7548936E-02	-0.5935065E-02	39
-0.4675679E-02	-0.3705234E-02	-0.2968737E-02	-0.2389941E-02	-0.1862353E-02	40
-0.1335975E-02	-0.6751183E-03	-0.3205158E-03			41
NE	010 1 72 69	0.40000	0.0	0.43320 0.73081	42
20 40 60 160 160 160 160 160 160 160					43
0.2054696E-02	0.4109390E-02	0.6164081E-02	0.8218773E-02	0.1027346E-01	44
0.1232816E-01	0.1438285E-01	0.1643754E-01	0.1849223E-01	0.2054692E-01	45
0.2260161E-01	0.2465630E-01	0.2671099E-01	0.2876569E-01	0.3082038E-01	46
0.3287507E-01	0.3492976E-01	0.3698445E-01	0.3903914E-01	0.4109383E-01	47
0.4520322E-01	0.4931261E-01	0.5342200E-01	0.5753139E-01	0.6164078E-01	48
0.6575012E-01	0.6985950E-01	0.7396889E-01	0.7807827E-01	0.8218765E-01	49
0.8629704E-01	0.9040642E-01	0.9451580E-01	0.9862518E-01	0.1027346E+00	50
0.1068439E+00	0.1109533E+00	0.1150627E+00	0.1191721E+00	0.1232815E+00	51
0.1315002E+00	0.1397190E+00	0.1479378E+00	0.1561565E+00	0.1643753E+00	52
0.1725941E+00	0.1808128E+00	0.1890316E+00	0.1972504E+00	0.2054691E+00	53
0.2136879E+00	0.2219067E+00	0.2301254E+00	0.2383442E+00	0.2465630E+00	54
0.2547817E+00	0.2630005E+00	0.2712193E+00	0.2794380E+00	0.2876568E+00	55
0.3040943E+00	0.3205318E+00	0.3369694E+00	0.3534069E+00	0.3698444E+00	56
0.3862820E+00	0.4027195E+00	0.4191570E+00	0.4355946E+00	0.4520321E+00	57
0.4684696E+00	0.4849072E+00				58
-0.9694691E+04	-0.4827574E+04	-0.3205081E+04	-0.2393760E+04	-0.1906919E+04	59
-0.1582328E+04	-0.1350458E+04	-0.1176544E+04	-0.1041272E+04	-0.9330547E+03	60
-0.8445154E+03	-0.7707383E+03	-0.7083184E+03	-0.6548245E+03	-0.6084727E+03	61
-0.5679255E+03	-0.5321599E+03	-0.5003799E+03	-0.4719570E+03	-0.4463884E+03	62
-0.4022603E+03	-0.3655332E+03	-0.3345020E+03	-0.3079480E+03	-0.2849773E+03	63
-0.2649182E+03	-0.2472579E+03	-0.2315963E+03	-0.2176178E+03	-0.2050696E+03	64
-0.1937471E+03	-0.1834826E+03	-0.1741375E+03	-0.1655964E+03	-0.1577623E+03	65
-0.1505529E+03	-0.1438982E+03	-0.1377384E+03	-0.1320216E+03	-0.1267030E+03	66
-0.1171092E+03	-0.1086993E+03	-0.1012729E+03	-0.9467226E+02	-0.8877127E+02	67
-0.8346828E+02	-0.7868033E+02	-0.7433910E+02	-0.7038782E+02	-0.6677904E+02	68
-0.6347263E+02	-0.6043454E+02	-0.5763564E+02	-0.5505083E+02	-0.5265831E+02	69
-0.5043915E+02	-0.4837672E+02	-0.4645638E+02	-0.4466516E+02	-0.4299158E+02	70
-0.3995744E+02	-0.3728436E+02	-0.3491637E+02	-0.3280814E+02	-0.3092279E+02	71
-0.2923012E+02	-0.2770522E+02	-0.2632742E+02	-0.2507945E+02	-0.2394675E+02	72
-0.2291695E+02	-0.2197952E+02				73
0.2975518E-01	0.1142313E+00	0.2466817E+00	0.4209120E+00	0.6312420E+00	74
0.8724714E+00	0.1139846E+01	0.1429028E+01	0.1736062E+01	0.2057357E+01	75
0.2389649E+01	0.2729987E+01	0.3075704E+01	0.3424397E+01	0.3773910E+01	76
0.4122313E+01	0.4467883E+01	0.4809093E+01	0.5144590E+01	0.5473190E+01	77
0.6105685E+01	0.6699875E+01	0.7250917E+01	0.7755533E+01	0.8211730E+01	78
0.8618584E+01	0.8976037E+01	0.9276437E+01	0.9545879E+01	0.9761108E+01	79
0.9932391E+01	0.1006194E+02	0.1015215E+02	0.1020552E+02	0.1022460E+02	80
0.1021198E+02	0.1017021E+02	0.1010181E+02	0.1000925E+02	0.9894886E+01	81
0.9609775E+01	0.9263420E+01	0.8870938E+01	0.8445575E+01	0.7998744E+01	82
0.7540126E+01	0.7077803E+01	0.6618404E+01	0.6167270E+01	0.5728602E+01	83
0.5305622E+01	0.4900701E+01	0.4515493E+01	0.4151058E+01	0.3807956E+01	84
0.3486343E+01	0.3186051E+01	0.2906652E+01	0.2647525E+01	0.2407896E+01	85
0.1983549E+01	0.1625896E+01	0.1326861E+01	0.1078561E+01	0.8736241E+00	86
0.7053668E+00	0.5678670E+00	0.4559672E+00	0.3652385E+00	0.2919204E+00	87
0.2328500E+00	0.1853884E+00				88



MG	012	2	76	73	-0.40000	0.0	0.0	0.47000	0.72913	89
	20	40	60	160	160	160	160	160	160	90
	0.1933543E-02	0.3867085E-02	0.5800623E-02	0.7734161E-02	0.9667698E-02					91
	0.1160124E-01	0.1353477E-01	0.1546831E-01	0.1740185E-01	0.1933539E-01					92
	0.2126892E-01	0.2320246E-01	0.2513600E-01	0.2706954E-01	0.2900307E-01					93
	0.3093661E-01	0.3287015E-01	0.3480368E-01	0.3673722E-01	0.3867076E-01					94
	0.4253784E-01	0.4640492E-01	0.5027201E-01	0.5413909E-01	0.5800617E-01					95
	0.6187325E-01	0.6574029E-01	0.6960732E-01	0.7347435E-01	0.7734138E-01					96
	0.8120841E-01	0.8507544E-01	0.8894247E-01	0.9280950E-01	0.9667653E-01					97
	0.1005436E+00	0.1044106E+00	0.1082776E+00	0.1121446E+00	0.1160117E+00					98
	0.1237457E+00	0.1314798E+00	0.1392139E+00	0.1469479E+00	0.1546820E+00					99
	0.1624160E+00	0.1701501E+00	0.1778842E+00	0.1856182E+00	0.1933523E+00					100
	0.2010863E+00	0.2088204E+00	0.2165545E+00	0.2242885E+00	0.2320226E+00					101
	0.2397566E+00	0.2474907E+00	0.2552248E+00	0.2629588E+00	0.2706929E+00					102
	0.2861611E+00	0.3016294E+00	0.3170976E+00	0.3325658E+00	0.3480341E+00					103
	0.3635023E+00	0.3789706E+00	0.3944388E+00	0.4099070E+00	0.4253753E+00					104
	0.4408435E+00	0.4563118E+00	0.4717800E+00	0.4872482E+00	0.5027165E+00					105
	0.5181847E+00									106
	-0.1235791E+05	-0.6151395E+04	-0.4082400E+04	-0.3047810E+04	-0.2427000E+04					107
	-0.2013093E+04	-0.1717426E+04	-0.1495669E+04	-0.1323191E+04	-0.1185215E+04					108
	-0.1072334E+04	-0.9782803E+03	-0.8987109E+03	-0.8305254E+03	-0.7714485E+03					109
	-0.7197749E+03	-0.6741995E+03	-0.6337068E+03	-0.5974961E+03	-0.5649253E+03					110
	-0.5087217E+03	-0.4619558E+03	-0.4224521E+03	-0.3886562E+03	-0.3594275E+03					111
	-0.3339092E+03	-0.3114468E+03	-0.2915303E+03	-0.2737568E+03	-0.2578042E+03					112
	-0.2434111E+03	-0.2303642E+03	-0.2184866E+03	-0.2076313E+03	-0.1976746E+03					113
	-0.1885119E+03	-0.1800540E+03	-0.1722247E+03	-0.1649581E+03	-0.1581972E+03					114
	-0.1460006E+03	-0.1353075E+03	-0.1258639E+03	-0.1174695E+03	-0.1099650E+03					115
	-0.1032213E+03	-0.9713354E+02	-0.9161501E+02	-0.8659364E+02	-0.8200900E+02					116
	-0.7780997E+02	-0.7395287E+02	-0.7040030E+02	-0.6711993E+02	-0.6408366E+02					117
	-0.6126698E+02	-0.5864844E+02	-0.5620914E+02	-0.5393243E+02	-0.5180360E+02					118
	-0.4793890E+02	-0.4452713E+02	-0.4149831E+02	-0.3879622E+02	-0.3637531E+02					119
	-0.3419826E+02	-0.3223416E+02	-0.3045724E+02	-0.2884576E+02	-0.2738127E+02					120
	-0.2604794E+02	-0.2483218E+02	-0.2372220E+02	-0.2270770E+02	-0.2177972E+02					121
	-0.2093042E+02									122
	0.4580327E-01	0.1749096E+00	0.3757172E+00	0.6376935E+00	0.9512933E+00					123
	0.1307882E+01	0.1699668E+01	0.2119631E+01	0.2561462E+01	0.3019513E+01					124
	0.3488731E+01	0.3964619E+01	0.4443184E+01	0.4920897E+01	0.5394655E+01					125
	0.5861739E+01	0.6319783E+01	0.6766746E+01	0.7200876E+01	0.7620689E+01					126
	0.8412610E+01	0.9135054E+01	0.9783422E+01	0.1035542E+02	0.1085061E+02					127
	0.1126999E+02	0.1161568E+02	0.1189066E+02	0.1209854E+02	0.1224336E+02					128
	0.1232944E+02	0.1236126E+02	0.1234337E+02	0.1228029E+02	0.1217645E+02					129
	0.1203616E+02	0.1186354E+02	0.1166253E+02	0.1143685E+02	0.1119000E+02					130
	0.1064555E+02	0.1005243E+02	0.9430264E+01	0.8795227E+01	0.8160419E+01					131
	0.7536180E+01	0.6930467E+01	0.6349185E+01	0.5796524E+01	0.5275245E+01					132
	0.4786945E+01	0.4332289E+01	0.3911202E+01	0.3523043E+01	0.3166745E+01					133
	0.2840932E+01	0.2544016E+01	0.2274278E+01	0.2029923E+01	0.1809141E+01					134
	0.1431144E+01	0.1126569E+01	0.8829421E+00	0.6893017E+00	0.5362442E+00					135
	0.4158553E+00	0.3215727E+00	0.2480209E+00	0.1908406E+00	0.1465265E+00					136
	0.1122804E+00	0.8588272E-01	0.6558204E-01	0.5000329E-01	0.3807138E-01					137
	0.2894885E-01									138
	-0.1598589E+02									139

# F. RIG: SCF INPUT (TRIAL EIGENVALUES AND SYMMETRY CARDS)

0000100	0	1				
0000200	6,8,1,1,5,6,0,0,2,.05,1.					
0000300	2.		-60.9204			
0000400	2.		-92.6720			
0000500	S1	2.	-6.30841	.005	1	1 0
0000600	8	2		SIGMA EP		
0000700	0	1				
0000800	0	1	1	1.00000000		
0000900	1	1				
0001000	1	1	1	1.00000000		
0001100	2	1				
0001200	0	1	1	1.00000000		
0001300	2	1				
0001400	2	1	1	1.00000000		
0001500	0	1				
0001600	0	1	2	1.00000000		
0001700	1	1				

0001800	1	1	2	1.00000000			
0001900	0	1					
0002000	0	1	3	1.00000000			
0002100	1	1					
0002200	1	1	3	1.00000000			
0002300	S2	2.	-4.51048	.005	1	1	0
0002400	S3	2.	-2.88924	.005	1	1	0
0002420	S4	2.	-1.46411	.005	1	1	0
0002500	PI1	4.	-3.63858	.005	5	1	0
0002600	10	2	PI Z REP				
0002700	1	1					
0002800	0	1	1	1.00000000			
0002900	2	1					
0003000	1	1	1	1.00000000			
0003100	3	1					
0003200	0	1	1	1.00000000			
0003300	3	1					
0003400	2	1	1	1.00000000			
0003500	4	1					
0003600	1	1	1	1.00000000			
0003700	4	1					
0003800	3	1	1	1.00000000			
0003900	1	1					
0004000	0	1	2	1.00000000			
0004100	2	1					
0004200	1	1	2	1.00000000			
0004300	1	1					
0004400	0	1	3	1.00000000			
0004500	2	1					
0004600	1	1	3	1.00000000			
0004700	PI2	4.	-1.601967	.005	5	1	0

## REFERENCES

1. Ferrante, J.; and Pepper, S. V.: Production of Ne Auger Electrons by Ne + Bombardment of Mg and Al Surfaces. *Surface Sci.*, vol. 57, no. 1, July 1976, pp. 420-424.  
Pepper, S. V.; and Ferrante, J.: Comments on Auger Electron Production by Ne + Bombardment of Surfaces. *Surface Sci.*, vol. 88, no. 1, Oct. 3, 1979, pp. L1- L5.
2. Barat, M.; and Lichten, W.: Extension of the Electron-Promotion Model to Asymmetric Atomic Collisions. *Phys. Rev.*, vol. 6A, no. 1, July 1972, pp. 211-229.
3. Ferrante, J.; and Pepper, S. V.: Production of Mg and Al Auger Electrons by Noble Gas Ion Bombardment of Mg and Al Surfaces. *Surface Sci.*, vol. 58, no. 2, Aug. 1976, pp. 613-617.
4. Slater, J. C.; and Johnson, K. H.: Self-Consistent-Field  $X\alpha$  Cluster Method for Polyatomic Molecules and Solids. *Phys. Rev.*, vol. 5B, no. 3, Feb. 1972, pp. 844-853.
5. Johnson, K. H.: Scattered-Wave Theory of the Chemical Bond. *Advances in Quantum Chemistry*. Vol. 7. P. O. Lowdin, ed., Academic Press, Inc., 1973, pp. 143-185.
6. Slater, J. C.: *Quantum Theory of Molecules and Solids, The Self-Consistent Field for Molecules and Solids*. Vol. 4. McGraw-Hill Book Co., Inc., 1974, p. 101.
7. Johnson, K. H.: *Quantum Chemistry*. *Annual Review of Physical Chemistry*. Vol. 26. H. Eyring, A. J. Cristensen, and H. S. Johnson, eds., Annual Reviews, pp. 39-57.
8. Herman, F.; and Skillman, S.: *Atomic Structure Calculations*. Prentice Hall, Inc., 1963.



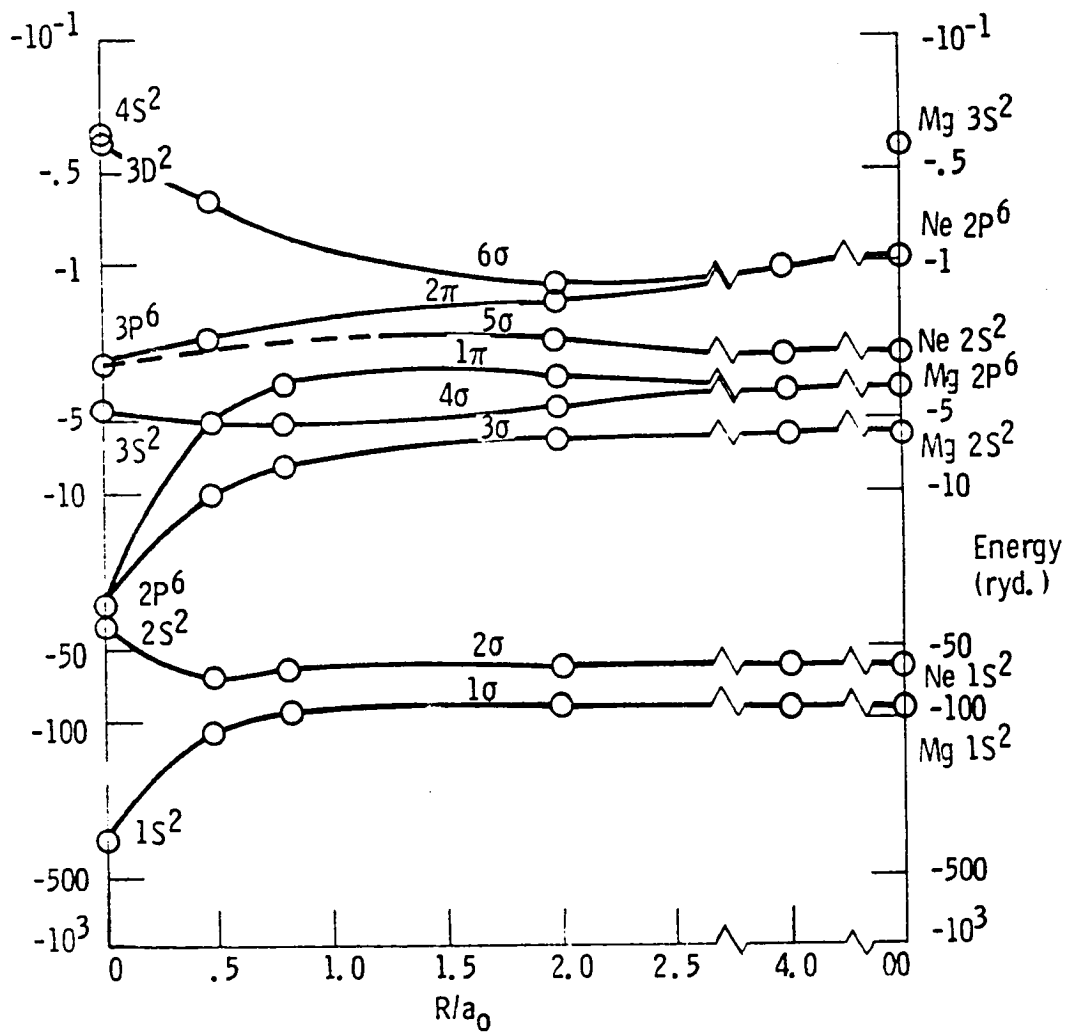


Figure 1. - Correlation diagram for Ne-Mg.

1. Report No. <b>NASA TM-81710</b>	2. Government Accession No.	3. Recipient's Catalog No.	
4. Title and Subtitle <b>THE SELF-CONSISTENT CALCULATION OF PSEUDO-MOLECULE ENERGY LEVELS, CONSTRUCTION OF ENERGY LEVEL CORRELATION DIAGRAMS AND AN AUTOMATED COMPUTATIONAL SYSTEM FOR SCF-X<math>\alpha</math>-SW CALCULATIONS</b>		5. Report Date <b>March 1981</b>	
		6. Performing Organization Code <b>506-53-12</b>	
7. Author(s) <b>Herbert Schlosser</b>		8. Performing Organization Report No. <b>E-740</b>	
9. Performing Organization Name and Address <b>National Aeronautics and Space Administration Lewis Research Center Cleveland, Ohio 44135</b>		10. Work Unit No.	
		11. Contract or Grant No.	
12. Sponsoring Agency Name and Address <b>National Aeronautics and Space Administration Washington, D. C. 20546</b>		13. Type of Report and Period Covered <b>Technical Memorandum</b>	
		14. Sponsoring Agency Code	
15. Supplementary Notes  <b>Author's present address: Physics Department, Cleveland State University, Cleveland, Ohio.</b>			
16. Abstract  This work is concerned with the self-consistent calculation of the electronic energy levels of noble gas pseudomolecules formed when a metal surface is bombarded by noble gas ions and with the construction of energy level correlation diagrams as a function of interatomic spacing. The self-consistent-field $x\alpha$ scattered wave (SCF-X $\alpha$ -SW) method of Slater and Johnson is utilized. Preliminary results on the Ne-Mg system are given. An interactive $x\alpha$ programming system, which has been implemented on the LeRC IBM 370 computer, is described in detail. This automated system makes use of special PROCDEFS (procedure definitions) to minimize the data to be entered manually at a remote terminal. Listings of the special PROCDEFS and of typical input data are given.			
17. Key Words (Suggested by Author(s))  <b>Pseudomolecules                      X-alpha method Correlation diagrams              Magnesium Neon</b>		18. Distribution Statement  <b>Unclassified - unlimited STAR Category 72</b>	
19. Security Classif. (of this report) <b>Unclassified</b>	20. Security Classif. (of this page) <b>Unclassified</b>	21. No. of Pages	22. Price*



National Aeronautics and  
Space Administration

Washington, D.C.  
20546

Official Business

Penalty for Private Use, \$300

SPECIAL FOURTH CLASS MAIL  
BOOK

Postage and Fees Paid  
National Aeronautics and  
Space Administration  
NASA-451



**NASA**

POSTMASTER: If Undeliverable (Section 158  
Postal Manual) Do Not Return

---